AN INFORMATION-THEORETIC TOOL FOR PROPERTY PREDICTION OF RANDOM MICROSTRUCTURES

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An information-theoretic tool for the extraction of microstructure information during deformation processes of multiphase materials and the simultaneous evaluation of homogenized-properties will be discussed. Microstructures can be considered as realizations of specific stochastic processes and in many practical instances the description of microstructure could be specified only using certain lower-order correlation functions. Hence, we do not have a deterministic characterization of the microstructure and this necessitates the need for a stochastic analysis. This in turn requires techniques to be employed to generate samples of the microstructure from limited information. An information-theoretic approach would be developed to generate these samples. Further, the critical interest lies in simultaneously obtaining statistics of homogenized-properties. Algorithms will be discussed for developing effective properties for this stochastic description of microstructures.

During the microstructure evolution process, information regarding the microstructure is updated at each time step using the evolved correlation functions. The information extracted from the microstructure is in the form of morphological features utilizing indicator functions. For instance, one of the commonly used lower-order descriptors is the two-point correlation function which characterizes the spatial correlation of two randomly selected points. The information theoretic tool takes as input this set of probabilistic information about the random field describing the microstructure (in the form of lower-order descriptors) and generates samples of microstructures that represent this given information. This is based on the “Maximum Entropy Principle”, which states that the entropy (of the set of microstructural indicators) needs to be as high as possible in the unconstrained dimensions while ensuring that the constraints imposed by the available information are satisfied. These samples of the microstructure will be interrogated at each time step to evaluate their homogenized-properties. Numerical examples explicating this scheme for a given instance of morphological features will be discussed.